



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:56 PM GMT

PDB ID : 3DB1
Title : Crystal structure of the 2H-phosphatase domain of Sts-2 in complex with phosphate
Authors : Nassar, N.; Chen, Y.; Carpino, N.
Deposited on : 2008-05-30
Resolution : 2.77 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

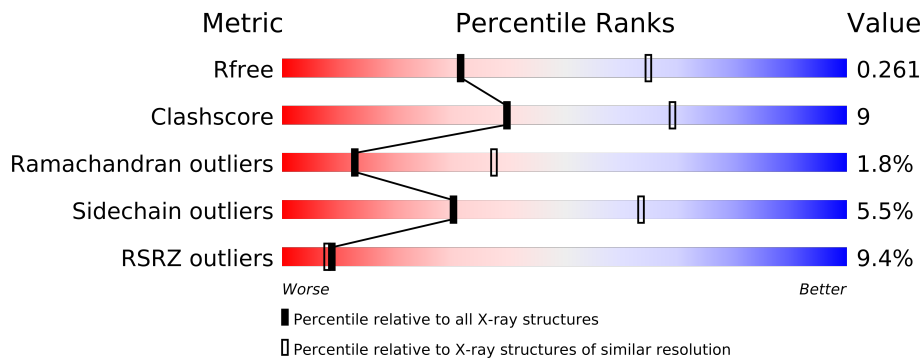
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.77 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2193 (2.80-2.76)
Clashscore	79885	2751 (2.80-2.76)
Ramachandran outliers	78287	2699 (2.80-2.76)
Sidechain outliers	78261	2701 (2.80-2.76)
RSRZ outliers	66119	2196 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	273	
1	B	273	
1	C	273	
1	D	273	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	D	4	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8421 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

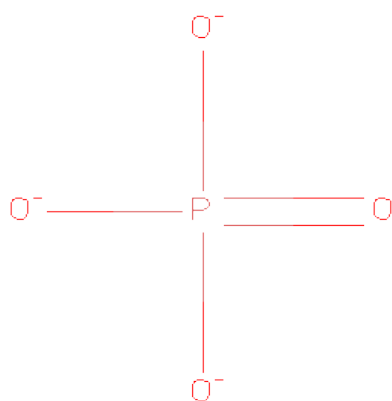
- Molecule 1 is a protein called STS-2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2115	1338	375	387	15			
1	B	263	Total	C	N	O	S	0	0	0
			2088	1321	371	381	15			
1	C	264	Total	C	N	O	S	0	0	0
			2096	1327	372	382	15			
1	D	265	Total	C	N	O	S	0	0	0
			2102	1330	373	384	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	ALA	-	EXPRESSION TAG	UNP Q8BX41
A	351	MET	-	EXPRESSION TAG	UNP Q8BX41
A	352	GLY	-	EXPRESSION TAG	UNP Q8BX41
A	353	SER	-	EXPRESSION TAG	UNP Q8BX41
A	364	ILE	VAL	CONFLICT	UNP Q8BX41
B	350	ALA	-	EXPRESSION TAG	UNP Q8BX41
B	351	MET	-	EXPRESSION TAG	UNP Q8BX41
B	352	GLY	-	EXPRESSION TAG	UNP Q8BX41
B	353	SER	-	EXPRESSION TAG	UNP Q8BX41
B	364	ILE	VAL	CONFLICT	UNP Q8BX41
C	350	ALA	-	EXPRESSION TAG	UNP Q8BX41
C	351	MET	-	EXPRESSION TAG	UNP Q8BX41
C	352	GLY	-	EXPRESSION TAG	UNP Q8BX41
C	353	SER	-	EXPRESSION TAG	UNP Q8BX41
C	364	ILE	VAL	CONFLICT	UNP Q8BX41
D	350	ALA	-	EXPRESSION TAG	UNP Q8BX41
D	351	MET	-	EXPRESSION TAG	UNP Q8BX41
D	352	GLY	-	EXPRESSION TAG	UNP Q8BX41
D	353	SER	-	EXPRESSION TAG	UNP Q8BX41
D	364	ILE	VAL	CONFLICT	UNP Q8BX41

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			4	3	1		

- Molecule 3 is water.

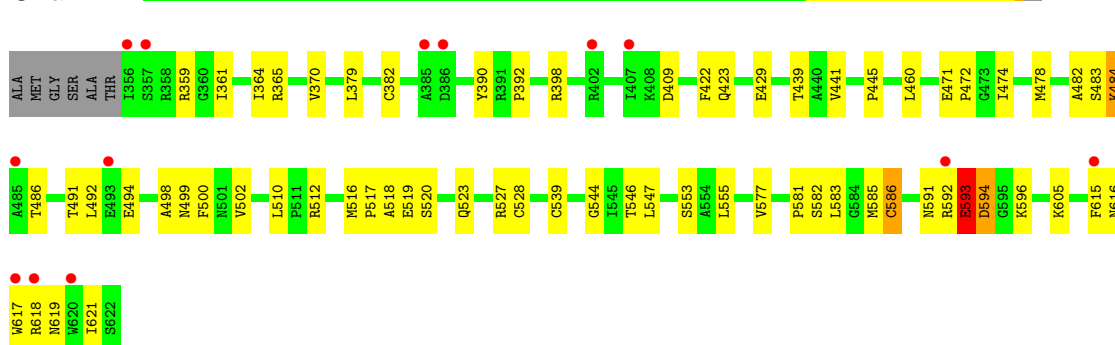
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		
3	C	2	Total	O	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

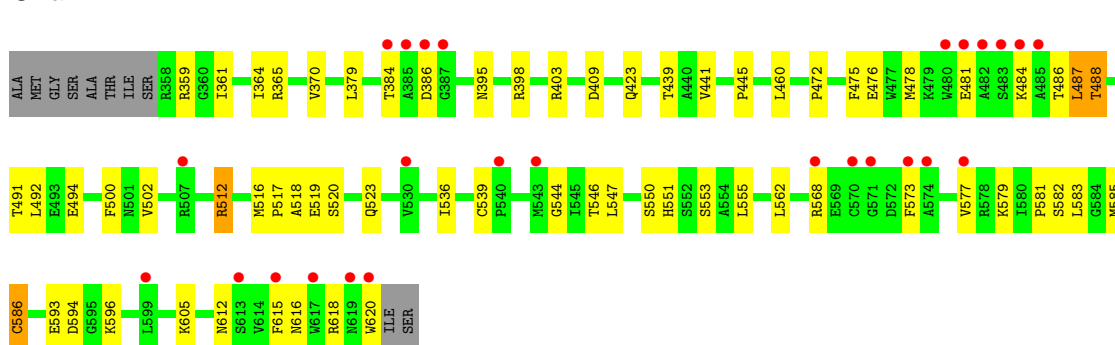
• Molecule 1: STS-2 protein

Chain A:



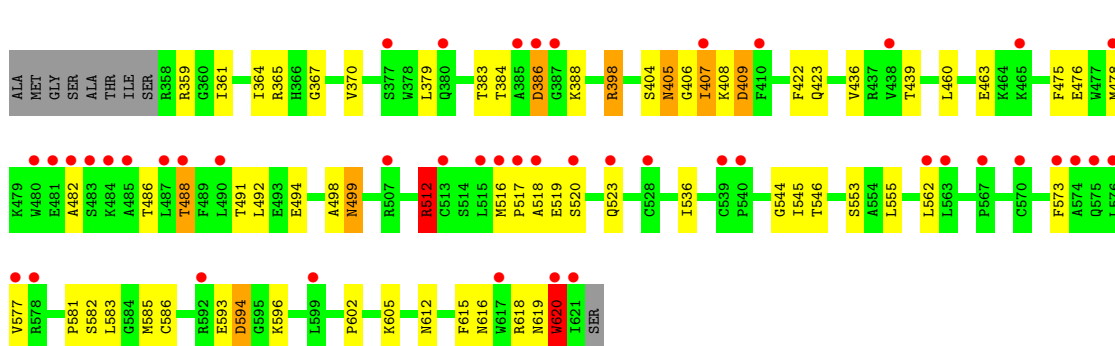
• Molecule 1: STS-2 protein

Chain B:



• Molecule 1: STS-2 protein

Chain C:



● Molecule 1: STS-2 protein

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.08Å 117.03Å 121.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.69 – 2.77 43.70 – 2.77	Depositor EDS
% Data completeness (in resolution range)	96.9 (43.69-2.77) 97.0 (43.70-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.270 0.235 , 0.261	Depositor DCC
R_{free} test set	1429 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.7	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 27988 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8421	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8502e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.78	2/2163 (0.1%)	0.87	5/2929 (0.2%)
1	B	0.66	1/2136 (0.0%)	0.81	5/2894 (0.2%)
1	C	0.63	0/2144	0.69	4/2905 (0.1%)
1	D	0.67	1/2150 (0.0%)	0.74	5/2913 (0.2%)
All	All	0.69	4/8593 (0.0%)	0.78	19/11641 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	586	CYS	CB-SG	-7.40	1.69	1.82
1	B	586	CYS	CB-SG	-7.00	1.70	1.82
1	D	372	GLN	CG-CD	5.53	1.63	1.51
1	A	382	CYS	CB-SG	-5.07	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	ARG	NE-CZ-NH2	16.58	128.59	120.30
1	A	512	ARG	NE-CZ-NH1	-15.79	112.40	120.30
1	B	359	ARG	NE-CZ-NH2	15.65	128.12	120.30
1	B	359	ARG	NE-CZ-NH1	-15.48	112.56	120.30
1	A	512	ARG	CD-NE-CZ	8.47	135.46	123.60
1	D	512	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	B	512	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	512	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	359	ARG	CD-NE-CZ	7.11	133.56	123.60
1	A	359	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	359	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	C	359	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	C	512	ARG	NE-CZ-NH1	6.60	123.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	512	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	359	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	359	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	359	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	512	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	365	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2115	0	2114	47	0
1	B	2088	0	2086	43	0
1	C	2096	0	2097	41	0
1	D	2102	0	2102	51	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
All	All	8421	0	8399	159	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (159) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:594:ASP:HB3	1:B:596:LYS:HG2	1.43	0.99
1:D:403:ARG:NH2	1:D:488:THR:O	2.01	0.93
1:A:616:ASN:HD21	1:A:619:ASN:CG	1.82	0.80
1:A:594:ASP:HB3	1:A:596:LYS:HG2	1.64	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:617:TRP:O	1:A:621:ILE:HG23	1.84	0.78
1:A:618:ARG:O	1:A:621:ILE:HG12	1.87	0.74
1:C:478:MET:HB2	1:C:519:GLU:HG2	1.69	0.74
1:A:594:ASP:CB	1:A:596:LYS:HG2	2.18	0.73
1:D:619:ASN:O	1:D:620:TRP:HB2	1.90	0.72
1:B:615:PHE:HB2	1:D:581:PRO:HG3	1.73	0.71
1:D:594:ASP:CB	1:D:596:LYS:HG2	2.21	0.71
1:B:616:ASN:HD21	1:B:618:ARG:HB2	1.55	0.70
1:C:409:ASP:OD2	1:C:488:THR:HG21	1.91	0.69
1:A:478:MET:HB2	1:A:519:GLU:HG2	1.75	0.69
1:D:478:MET:HB2	1:D:519:GLU:HG2	1.75	0.69
1:B:478:MET:HB2	1:B:519:GLU:HG2	1.76	0.68
1:B:581:PRO:HG3	1:D:615:PHE:HB2	1.76	0.67
1:A:616:ASN:ND2	1:A:619:ASN:CG	2.48	0.66
1:D:594:ASP:HB3	1:D:596:LYS:HG2	1.76	0.66
1:B:484:LYS:HA	1:B:487:LEU:HD22	1.75	0.66
1:B:594:ASP:CB	1:B:596:LYS:HG2	2.23	0.66
1:A:615:PHE:CZ	1:A:617:TRP:HB2	2.30	0.66
1:C:492:LEU:H	1:C:492:LEU:HD12	1.62	0.65
1:A:592:ARG:NH1	1:A:592:ARG:HA	2.13	0.64
1:A:484:LYS:HD3	1:D:483:SER:H	1.63	0.63
1:B:579:LYS:NZ	1:D:620:TRP:CZ2	2.66	0.63
1:B:581:PRO:CG	1:D:615:PHE:HB2	2.29	0.63
1:C:404:SER:O	1:C:406:GLY:N	2.32	0.62
1:D:491:THR:OG1	1:D:494:GLU:HG3	1.99	0.62
1:D:619:ASN:O	1:D:620:TRP:CB	2.49	0.61
1:A:492:LEU:HD12	1:A:492:LEU:H	1.65	0.60
1:A:616:ASN:ND2	1:A:619:ASN:HB2	2.17	0.59
1:C:364:ILE:HG12	1:C:585:MET:HG2	1.85	0.59
1:B:612:ASN:HD21	1:D:582:SER:H	1.52	0.58
1:D:555:LEU:HD23	1:D:586:CYS:HB2	1.85	0.57
1:D:492:LEU:HD12	1:D:492:LEU:H	1.69	0.57
1:B:492:LEU:H	1:B:492:LEU:HD12	1.68	0.57
1:B:484:LYS:HA	1:B:487:LEU:CD2	2.34	0.57
1:A:592:ARG:HA	1:A:592:ARG:CZ	2.34	0.57
1:A:482:ALA:C	1:A:484:LYS:H	2.08	0.57
1:C:482:ALA:HB1	1:C:486:THR:OG1	2.04	0.56
1:B:361:ILE:HD13	1:B:546:THR:HB	1.87	0.56
1:C:491:THR:OG1	1:C:494:GLU:HG3	2.04	0.56
1:B:553:SER:HB2	1:B:573:PHE:HZ	1.70	0.55
1:C:553:SER:HB2	1:C:573:PHE:HZ	1.71	0.55
1:B:403:ARG:NH2	1:B:488:THR:O	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:423:GLN:HB3	1:C:583:LEU:HD23	1.89	0.54
1:D:520:SER:OG	1:D:523:GLN:HG3	2.08	0.54
1:D:364:ILE:HG12	1:D:585:MET:HG2	1.88	0.54
1:C:384:THR:OG1	1:C:386:ASP:HB3	2.07	0.54
1:C:594:ASP:HB2	1:C:596:LYS:HG2	1.89	0.54
1:A:491:THR:OG1	1:A:494:GLU:HG3	2.07	0.54
1:A:484:LYS:HD2	1:A:484:LYS:C	2.29	0.53
1:A:361:ILE:HD13	1:A:546:THR:HB	1.91	0.53
1:A:555:LEU:HD23	1:A:586:CYS:HB2	1.91	0.53
1:B:581:PRO:CD	1:D:615:PHE:HB2	2.39	0.52
1:A:364:ILE:HG12	1:A:585:MET:HG2	1.90	0.52
1:A:616:ASN:ND2	1:A:619:ASN:CB	2.72	0.52
1:A:618:ARG:NH1	1:C:602:PRO:HD3	2.25	0.52
1:B:384:THR:OG1	1:B:386:ASP:HB3	2.10	0.52
1:B:615:PHE:HB2	1:D:581:PRO:CG	2.39	0.52
1:B:520:SER:OG	1:B:523:GLN:HG3	2.10	0.52
1:A:615:PHE:HB2	1:C:581:PRO:HG3	1.92	0.52
1:D:616:ASN:HD21	1:D:619:ASN:HB2	1.75	0.52
1:C:404:SER:C	1:C:406:GLY:H	2.14	0.52
1:D:539:CYS:SG	1:D:539:CYS:O	2.67	0.52
1:D:594:ASP:HB2	1:D:596:LYS:HG2	1.92	0.51
1:B:395:ASN:HB2	1:D:608:THR:O	2.10	0.51
1:C:594:ASP:C	1:C:596:LYS:H	2.13	0.51
1:B:491:THR:OG1	1:B:494:GLU:HG3	2.10	0.51
1:A:593:GLU:O	1:A:594:ASP:C	2.50	0.51
1:B:364:ILE:HG12	1:B:585:MET:HG2	1.93	0.51
1:C:406:GLY:C	1:C:408:LYS:N	2.62	0.51
1:A:484:LYS:HB2	1:D:483:SER:HB3	1.92	0.50
1:A:553:SER:HA	1:A:577:VAL:HG11	1.93	0.50
1:A:472:PRO:HB2	1:A:510:LEU:O	2.11	0.50
1:D:593:GLU:O	1:D:595:GLY:N	2.44	0.50
1:C:618:ARG:C	1:C:620:TRP:H	2.15	0.49
1:D:361:ILE:HD13	1:D:546:THR:HB	1.94	0.49
1:C:555:LEU:HD23	1:C:586:CYS:HB2	1.94	0.49
1:B:555:LEU:HD23	1:B:586:CYS:HB2	1.94	0.49
1:B:439:THR:HG23	1:B:544:GLY:HA3	1.95	0.49
1:B:423:GLN:HB3	1:B:583:LEU:HD23	1.94	0.48
1:C:405:ASN:O	1:C:408:LYS:HG2	2.13	0.48
1:D:553:SER:HA	1:D:577:VAL:HG11	1.96	0.48
1:B:568:ARG:HH22	1:D:621:ILE:HG23	1.78	0.48
1:C:594:ASP:CB	1:C:596:LYS:HG2	2.43	0.48
1:D:593:GLU:O	1:D:594:ASP:C	2.51	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:539:CYS:O	1:B:539:CYS:SG	2.72	0.48
1:C:361:ILE:HD13	1:C:546:THR:HB	1.96	0.47
1:A:582:SER:H	1:C:612:ASN:HD21	1.63	0.47
1:C:439:THR:HG23	1:C:544:GLY:HA3	1.96	0.47
1:B:579:LYS:NZ	1:D:620:TRP:CE2	2.76	0.47
1:B:616:ASN:ND2	1:B:618:ARG:HB2	2.28	0.47
1:A:423:GLN:HB3	1:A:583:LEU:HD23	1.97	0.47
1:D:369:ARG:HG3	1:D:372:GLN:HB2	1.96	0.47
1:D:436:VAL:HB	1:D:545:ILE:HD12	1.97	0.47
1:D:536:ILE:HD11	1:D:562:LEU:HD11	1.98	0.46
1:D:486:THR:HG21	1:D:515:LEU:HB2	1.97	0.46
1:C:367:GLY:HA2	1:C:582:SER:HB3	1.98	0.46
1:A:581:PRO:HG3	1:C:615:PHE:HB2	1.99	0.45
1:A:500:PHE:O	1:A:502:VAL:N	2.50	0.45
1:C:475:PHE:CG	1:C:476:GLU:N	2.85	0.45
1:C:383:THR:HA	1:C:388:LYS:O	2.16	0.45
1:C:404:SER:C	1:C:406:GLY:N	2.70	0.45
1:C:463:GLU:N	1:C:463:GLU:OE1	2.47	0.45
1:D:445:PRO:HD3	1:D:472:PRO:HA	1.98	0.44
1:B:475:PHE:CG	1:B:476:GLU:N	2.85	0.44
1:B:484:LYS:H	1:B:517:PRO:HB3	1.82	0.44
1:A:484:LYS:HB2	1:D:483:SER:CB	2.48	0.44
1:B:500:PHE:O	1:B:502:VAL:N	2.50	0.44
1:A:527:ARG:HG3	1:A:528:CYS:N	2.32	0.44
1:B:445:PRO:HD3	1:B:472:PRO:HA	1.99	0.44
1:D:463:GLU:OE1	1:D:463:GLU:N	2.51	0.44
1:D:439:THR:HG23	1:D:544:GLY:HA3	2.00	0.44
1:C:553:SER:HA	1:C:577:VAL:HG11	2.00	0.44
1:D:475:PHE:CG	1:D:476:GLU:N	2.86	0.44
1:C:436:VAL:HB	1:C:545:ILE:HD12	1.99	0.44
1:A:482:ALA:C	1:A:484:LYS:N	2.70	0.43
1:C:520:SER:OG	1:C:523:GLN:HG3	2.18	0.43
1:A:439:THR:HG23	1:A:544:GLY:HA3	2.00	0.43
1:A:520:SER:OG	1:A:523:GLN:HG3	2.19	0.43
1:C:409:ASP:OD2	1:C:488:THR:CG2	2.65	0.42
1:A:539:CYS:SG	1:A:539:CYS:O	2.77	0.42
1:B:536:ILE:HD11	1:B:562:LEU:HD11	2.01	0.42
1:B:395:ASN:CB	1:D:608:THR:O	2.67	0.42
1:C:536:ILE:HD11	1:C:562:LEU:HD11	2.02	0.42
1:A:445:PRO:HD3	1:A:472:PRO:HA	2.01	0.42
1:A:615:PHE:HZ	1:A:617:TRP:HB2	1.82	0.42
1:C:616:ASN:HD21	1:C:618:ARG:HB2	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:620:TRP:CE3	1:C:620:TRP:HA	2.55	0.42
1:A:471:GLU:O	1:A:474:ILE:HG12	2.19	0.42
1:B:553:SER:HA	1:B:577:VAL:HG11	2.01	0.42
1:A:390:TYR:O	1:A:392:PRO:HD3	2.20	0.41
1:D:412:ASN:HB2	1:D:488:THR:HG21	2.02	0.41
1:A:591:ASN:HD22	1:A:596:LYS:NZ	2.17	0.41
1:B:476:GLU:HG2	1:B:481:GLU:OE2	2.20	0.41
1:B:582:SER:N	1:D:612:ASN:HD21	2.18	0.41
1:B:550:SER:OG	1:B:551:HIS:N	2.51	0.41
1:A:516:MET:C	1:A:518:ALA:H	2.22	0.41
1:C:516:MET:C	1:C:518:ALA:H	2.23	0.41
1:A:439:THR:CG2	1:A:544:GLY:HA3	2.50	0.41
1:C:512:ARG:H	1:C:512:ARG:HG2	1.65	0.41
1:D:367:GLY:HA2	1:D:582:SER:HB3	2.01	0.41
1:B:568:ARG:NH2	1:D:621:ILE:HG23	2.36	0.41
1:A:429:GLU:CD	1:C:398:ARG:HE	2.23	0.41
1:A:593:GLU:HG3	1:A:593:GLU:H	1.68	0.41
1:D:384:THR:OG1	1:D:386:ASP:HB3	2.21	0.41
1:D:441:VAL:O	1:D:441:VAL:HG23	2.20	0.41
1:B:516:MET:C	1:B:518:ALA:H	2.23	0.41
1:A:498:ALA:O	1:A:499:ASN:HB3	2.20	0.41
1:B:439:THR:CG2	1:B:544:GLY:HA3	2.51	0.40
1:B:582:SER:H	1:D:612:ASN:HD21	1.67	0.40
1:A:484:LYS:HD3	1:D:483:SER:N	2.35	0.40
1:D:516:MET:C	1:D:518:ALA:H	2.24	0.40
1:C:406:GLY:C	1:C:408:LYS:H	2.24	0.40
1:D:553:SER:HB2	1:D:573:PHE:HZ	1.85	0.40
1:C:498:ALA:O	1:C:499:ASN:HB3	2.21	0.40
1:D:498:ALA:O	1:D:499:ASN:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/273 (97%)	242 (91%)	18 (7%)	5 (2%)	12	35
1	B	261/273 (96%)	244 (94%)	17 (6%)	0	100	100
1	C	262/273 (96%)	240 (92%)	15 (6%)	7 (3%)	8	24
1	D	263/273 (96%)	248 (94%)	8 (3%)	7 (3%)	8	24
All	All	1051/1092 (96%)	974 (93%)	58 (6%)	19 (2%)	13	37

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	405	ASN
1	D	620	TRP
1	C	386	ASP
1	C	619	ASN
1	C	620	TRP
1	D	386	ASP
1	D	483	SER
1	D	594	ASP
1	A	593	GLU
1	A	483	SER
1	A	594	ASP
1	D	593	GLU
1	D	499	ASN
1	A	486	THR
1	C	499	ASN
1	A	517	PRO
1	C	517	PRO
1	D	517	PRO
1	C	407	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/237 (98%)	221 (95%)	12 (5%)	32	67
1	B	230/237 (97%)	215 (94%)	15 (6%)	24	55
1	C	231/237 (98%)	217 (94%)	14 (6%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	232/237 (98%)	222 (96%)	10 (4%)	40	75
All	All	926/948 (98%)	875 (94%)	51 (6%)	30	63

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ARG
1	A	370	VAL
1	A	379	LEU
1	A	398	ARG
1	A	409	ASP
1	A	422	PHE
1	A	441	VAL
1	A	460	LEU
1	A	484	LYS
1	A	547	LEU
1	A	593	GLU
1	A	605	LYS
1	B	365	ARG
1	B	370	VAL
1	B	379	LEU
1	B	398	ARG
1	B	409	ASP
1	B	441	VAL
1	B	460	LEU
1	B	486	THR
1	B	487	LEU
1	B	488	THR
1	B	512	ARG
1	B	547	LEU
1	B	593	GLU
1	B	605	LYS
1	B	620	TRP
1	C	365	ARG
1	C	370	VAL
1	C	379	LEU
1	C	398	ARG
1	C	407	ILE
1	C	409	ASP
1	C	422	PHE
1	C	460	LEU
1	C	488	THR

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Mol	Chain	Res	Type
1	C	512	ARG
1	C	593	GLU
1	C	594	ASP
1	C	605	LYS
1	C	620	TRP
1	D	370	VAL
1	D	379	LEU
1	D	398	ARG
1	D	407	ILE
1	D	409	ASP
1	D	460	LEU
1	D	483	SER
1	D	512	ARG
1	D	547	LEU
1	D	605	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	ASN
1	A	612	ASN
1	A	616	ASN
1	B	612	ASN
1	C	601	ASN
1	C	612	ASN
1	D	405	ASN
1	D	612	ASN
1	D	616	ASN
1	D	619	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	1	-	4,4,4	0.20	0	6,6,6	0.33	0
2	PO4	C	3	-	4,4,4	0.23	0	6,6,6	0.32	0
2	PO4	D	4	-	1,3,4	4.70	1 (100%)	0,3,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	1	-	-	0/0/0/0	0/0/0/0
2	PO4	C	3	-	-	0/0/0/0	0/0/0/0
2	PO4	D	4	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	PO4	P-O1	4.70	1.52	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	267/273 (97%)	0.33	13 (4%)	28 30	31, 62, 90, 107	0
1	B	263/273 (96%)	0.66	26 (9%)	8 7	31, 62, 83, 105	4 (1%)
1	C	264/273 (96%)	0.98	45 (17%)	2 2	31, 62, 83, 100	6 (2%)
1	D	265/273 (97%)	0.44	16 (6%)	21 22	31, 62, 85, 114	0
All	All	1059/1092 (96%)	0.60	100 (9%)	9 8	31, 62, 86, 114	10 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	SER	18.0
1	C	482	ALA	12.7
1	C	485	ALA	12.6
1	C	481	GLU	12.2
1	C	483	SER	11.3
1	C	480	TRP	9.9
1	C	484	LYS	8.8
1	D	616	ASN	6.0
1	C	515	LEU	6.0
1	B	620	TRP	6.0
1	D	486	THR	5.5
1	D	620	TRP	5.4
1	B	573	PHE	5.3
1	C	573	PHE	5.3
1	A	618	ARG	5.3
1	C	574	ALA	5.3
1	B	617	TRP	5.2
1	B	485	ALA	4.5
1	B	482	ALA	4.3
1	B	540	PRO	4.2
1	A	617	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	617	TRP	4.2
1	B	386	ASP	4.1
1	D	487	LEU	4.0
1	C	570	CYS	3.9
1	A	485	ALA	3.9
1	C	621	ILE	3.8
1	B	484	LYS	3.8
1	B	385	ALA	3.7
1	C	620	TRP	3.7
1	B	574	ALA	3.6
1	C	385	ALA	3.6
1	B	387	GLY	3.5
1	D	621	ILE	3.4
1	B	571	GLY	3.4
1	A	357	SER	3.4
1	C	540	PRO	3.3
1	A	385	ALA	3.3
1	C	577	VAL	3.3
1	C	562	LEU	3.2
1	B	543	MET	3.2
1	C	528	CYS	3.2
1	D	402	ARG	3.2
1	C	576	LEU	3.2
1	C	387	GLY	3.2
1	C	478	MET	3.1
1	C	377	SER	3.1
1	C	617	TRP	3.1
1	B	530	VAL	3.1
1	D	615	PHE	3.0
1	A	615	PHE	3.0
1	C	516	MET	2.9
1	D	619	ASN	2.9
1	B	615	PHE	2.9
1	D	618	ARG	2.8
1	C	578	ARG	2.8
1	B	613	SER	2.8
1	B	481	GLU	2.7
1	A	620	TRP	2.7
1	D	599	LEU	2.7
1	A	592	ARG	2.7
1	C	465	LYS	2.7
1	C	513	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	599	LEU	2.6
1	B	384	THR	2.6
1	C	410	PHE	2.6
1	C	567	PRO	2.6
1	C	386	ASP	2.6
1	B	619	ASN	2.6
1	C	575	GLN	2.6
1	C	517	PRO	2.5
1	B	480	TRP	2.5
1	B	568	ARG	2.5
1	A	356	ILE	2.5
1	C	507	ARG	2.4
1	C	592	ARG	2.4
1	B	570	CYS	2.4
1	A	493	GLU	2.4
1	C	380	GLN	2.3
1	C	488	THR	2.3
1	A	407	ILE	2.3
1	B	577	VAL	2.3
1	D	465	LYS	2.3
1	C	518	ALA	2.3
1	D	435	GLY	2.3
1	C	563	LEU	2.3
1	A	386	ASP	2.3
1	C	407	ILE	2.2
1	A	402	ARG	2.1
1	C	539	CYS	2.1
1	D	563	LEU	2.1
1	B	507	ARG	2.1
1	D	485	ALA	2.1
1	C	438	VAL	2.1
1	C	487	LEU	2.1
1	D	576	LEU	2.0
1	C	490	LEU	2.0
1	C	520	SER	2.0
1	B	599	LEU	2.0
1	C	523	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	D	4	4/5	0.29	2.00	88,90,91,91	0
2	PO4	A	1	5/5	0.19	0.95	77,78,80,82	0
2	PO4	C	3	5/5	0.18	-0.34	99,100,101,102	0

6.5 Other polymers

There are no such residues in this entry.